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Editorial

Global Challenges: Opening up Chemistry, Pandemics, and Air Pollution

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As the first half of 2022 comes to a close, it is an interesting time to reflect on some recent trends. In many ways, the world is "opening" up again, with many colleagues going to their first "in person" conferences since the start of the pandemic in early 2020. A significant leap forward for open chemistry was made in 2021, with the Chemical Abstracts Service (CAS) Registry embracing a hybrid model and releasing half a million chemicals as the CAS Common Chemistry set under an open license.[1] *ACS Environmental Au* continues to develop as one of the key gold open access journals for publishing work on environmental topics.[2] The European Union has just launched the €400 million European Partnership for the Assessment of Risks from Chemicals (PARC), with ∼200 partners[3] and a whole work package on FAIR (Findable, Accessible, Interoperable, Reusable)[4,5] and Open[6] data. While these trends are cause for optimism, the CAS Registry continues to climb toward the 200 million chemical mark[7] and many of us were blown away by the sheer immensity of the chemical pollution problem at recent meetings. Other colleagues, e.g., those affected by war, by lockdowns, or with insufficient funds, are unable to share in the "post-pandemic" reopening, conferences, and travel. Others cannot afford the costs associated with open access or still do not see the benefits of open science.

Why the focus on these disjoint subjects? Both chemical pollution and the COVID-19 pandemic are global challenges requiring global solutions, where failure to act comes with a high price. Landrigan et al. estimated that 9 million premature deaths (16% of the global total) were caused by pollution in 2015.[8] Worldwide deaths directly due to the COVID-19 pandemic are already over 6 million[9] (January 2020 to May 2022). While public awareness is high, individuals often feel powerless to tackle global challenges—yet the pandemic has proven that individual actions can make an incredible collective difference. The same applies to open data and the exchange of research results—the collective benefit from many individual contributions can be extraordinary.

FAIR AND OPEN CHEMISTRY

The release of the CAS Common Chemistry data set[1] was heralded by many as a breakthrough for open science. Reflecting on my somewhat less enthusiastic personal reaction to this, I realized that my research career developed in an era where open chemical resources such as PubChem,[10,11] ChemSpider,[12] and the Human Metabolome Database (HMDB)[13,14] already existed. In the meantime, many more open resources have evolved and the awareness of the importance of open science and open access has increased, as highlighted by the inclusion of FAIR data work packages in initiatives such as PARC (more information on Open[6] and FAIR[4,5] in the cited references). I have been fortunate to work with many colleagues both (co-)developing and cross-integrating chemical content in various open resources. PubChem now counts 111 million chemicals from 861 data sources (May 29, 2022), while our own NORMAN Suspect List Exchange[15] (NORMAN-SLE) initiative launched in 2015 now includes 99 suspect lists from over 70 contributors (as of May 29, 2022). We are working with journals[16,17] and authors to help fill the gaps in open chemistry resources and look forward to working with *ACS Environmental Au* Editors and authors alike as the journal develops—both to help authors disseminate their research knowledge in a FAIR and Open manner and to help you, the readers, find it and reuse it. Again, *the collective benefit from many individual contributions can be incredible, even if not immediately obvious at the beginning.*

INCREASING AWARENESS OF AIR POLLUTION

Many articles in this issue of *ACS Environmental Au* have a common focus on air pollution, reflecting an increased interest in air quality as a result of the pandemic. Qiang Zhang and colleagues used a data fusion approach to investigate daily emission patterns from coal-fired power plants in China from 2017 to 2020. They combined information from the China coal-fired Power plant Emissions Database (CPED) and real-time measurements from continuous emission monitoring systems (CEMS) and compared the derived results with available statistics. The estimates captured high demand heating and cooling periods (winter and summer) as well as sudden increases (e.g., due to drought) or decreases (e.g., due to COVID-19 lockdowns). Seiji Yamazoe and colleagues introduce a system to directly capture CO_2 from air using liquid amine-solid carbamic acid phase separation. Their system using diamines bearing an aminocyclohexyl group exhibited a > 99% CO_2 removal efficiency with a 400 ppm of CO_2 flow system. Since isophorone diamine (IPDA) exhibits high efficiency under direct air capture conditions, a high CO_2

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capture rate is achieved and the system can be reused under adsorption−desorption cycles without degradation. The authors suggest that this phase separation system using IPDA is robust and durable for potentially practical use.

Yafang Cheng and colleagues revisit key driving processes affecting decadal trends of aerosol acidity in the United States (US). Their decade-long observations in the southeastern US challenges traditional thoughts that acidity increases with acidic emissions (e.g., SO_2, NO_x) and decreases with alkaline emissions (e.g., NH_3, dust). They investigated the relationship between increasing alkaline emissions and stable predicted aerosol acidity using a multiphase buffer theory. They predicted that aerosols would remain in the ammonia-buffered region until ∼2050 and that nitrate would remain largely in the gas phase. Manabu Shiraiwa and colleagues investigated the effects of acidity on reactive oxygen species (ROS) formation from secondary organic aerosols (SOA). ROS can contribute to aerosol-related health effects, causing oxidative stress *in vivo*. The authors used the electron paramagnetic resonance spin-trapping technique and a Diogenes chemiluminescence assay to discover distinct radical compositions and yields at different pH values (between 1 and 7.4) from the SOA generated by oxidation of the chemicals isoprene, α-terpineol, α-pinene, β-pinene, toluene, and naphthalene.

Meng Gao, Yike Guo, and colleagues demonstrated how optimization of the location of air quality monitoring sites would allow better reconstruction of $PM_{2.5}$ pollution in China. The authors applied five proper orthogonal decomposition (POD)-based sensor placement algorithms to optimize site locations. The best-performing algorithm was placed with site locations in regions where $PM_{2.5}$ pollution was most severe and reconstructed the $PM_{2.5}$ pollution more accurately than existing sites. Their study also demonstrated that existing monitoring efforts are likely to miss sources of pollution in less-populated regions. Finally, the focus on air pollution is further discussed in a Perspective by Hongchen Shen, Danmeng Shuai, and colleagues on the use of electrospun nanofibrous membranes for controlling airborne viruses (featured on the front cover of this issue). In an article clearly motivated by the pandemic, the authors argue that electrospun nanofibrous membranes do show promising results compared with conventional air filtration media due to their reduced pore size, large specific surface area and porosity, as well as retained surface and volume charges, but that standardized protocols must be established to assess the membrane performance for removing viral aerosols. They proposed a standardized aerosol filtration test system before future advancements were discussed.

FURTHER CHALLENGES REMAIN

Moving away from air, Shuxiao Wang and colleagues developed a high-resolution rice paddy mercury transport and transformation model for source apportionment of mercury species in Chinese rice grains. While 81% of the national average rice grain total mercury concentration was due to atmospheric mercury deposition (again showing the relevance of air pollution), almost 65% of the national average methylmercury concentrations in rice grains were due to soil mercury levels, mainly due to *in situ* methylation pathways. Extremely high rice grain methylmercury was observed in the Guizhou province and the surrounding areas, in regions of smelting, cement clinker production, or metal mining activities. Finally, in their Letter, Jessica DeYoung and Scott Shaw investigated the impact of fungi on the chemical environment and morphology of environmental films. Bulk properties of films were investigated over 2 and 12 months, revealing that fungi and fungal-associated aggregates covered approximately 14% of the surface after 12 months. A nutrient pool associated with the fungal hypha extended 50 μm orthogonally to the growth direction. Since the authors observed both long- and short-term effects on films, they recommended that fungal presence should be considered when analyzing environmental films.

SUMMARY

This Editorial has touched on only a couple of the global challenges we currently face. This issue of *ACS Environmental Au* contains gold open access articles contributing to the body of research helping address these challenges, with several articles focusing on air quality and the pandemic. The increasing awareness of the benefits of sharing data in an Open and FAIR manner is likewise helping develop chemical resources that benefit the research community and beyond, providing an essential foundation for tackling the challenge of chemical pollution and other sustainability issues. On behalf of the editorial team, I hope you enjoy this issue of *ACS Environmental Au* and look forward to hearing your thoughts on how the journal can support you on the issues of Open and FAIR data and environmental research more broadly.

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Notes

Views expressed in this editorial are those of the author and not necessarily the views of the ACS.

REFERENCES

(1) Jacobs, A.; Williams, D.; Hickey, K.; Patrick, N.; Williams, A. J.; Chalk, S.; McEwen, L.; Willighagen, E.; Walker, M.; Bolton, E.; Sinclair, G.; Sanford, A. CAS Common Chemistry in 2021: Expanding Access to Trusted Chemical Information for the Scientific Community. *J. Chem. Inf. Model.* **2022**, *62*, 2737.

(2) Jin, L.; Li, X. D. *ACS Environmental Au*—Gold Open Access toward a Greener Future. *ACS Environ. Au* **2022**, *2* (2), 74−76.

(3) Anses; European Commission. European Partnership for the Assessment of Risks from Chemicals (PARC). *Anses* (Anses - Agence nationale de sécurité sanitaire de l'alimentation, de l'environnement et du travail (French Agency for Food, Environmental and Occupational Health & Safety)). https://www.anses.fr/en/content/european-partnership-assessment-risks-chemicals-parc (accessed 2022-05-29).

(4) GO FAIR. FAIR Principles. https://www.go-fair.org/fair-principles/ (accessed 2021-03-23).

(5) The FAIRsharing Community; Sansone, S.-A.; McQuilton, P.; Rocca-Serra, P.; Gonzalez-Beltran, A.; Izzo, M.; Lister, A. L.; Thurston, M. FAIRsharing as a Community Approach to Standards, Repositories and Policies. *Nat. Biotechnol.* **2019**, *37* (4), 358−367.

(6) Suber, P.. Open Access Overview (definition, introduction). http://legacy.earlham.edu/~peters/fos/overview.htm (accessed 2021-07-03).

(7) American Chemical Society. CAS REGISTRY - The CAS Substance Collection. https://www.cas.org/cas-data/cas-registry (accessed 2022-02-02).

(8) Landrigan, P. J.; Fuller, R.; Acosta, N. J. R.; Adeyi, O.; Arnold, R.; Basu, N.; Baldé, A. B.; Bertollini, R.; Bose-O'Reilly, S.; Boufford, J. I.; Breysse, P. N.; Chiles, T.; Mahidol, C.; Coll-Seck, A. M.; Cropper,

https://doi.org/10.1021/acsenvironau.2c00032
ACS Environ. Au 2022, 2, 287−289

M. L.; Fobil, J.; Fuster, V.; Greenstone, M.; Haines, A.; Hanrahan, D.; Hunter, D.; Khare, M.; Krupnick, A.; Lanphear, B.; Lohani, B.; Martin, K.; Mathiasen, K. V.; McTeer, M. A.; Murray, C. J. L.; Ndahimananjara, J. D.; Perera, F.; Potočnik, J.; Preker, A. S.; Ramesh, J.; Rockström, J.; Salinas, C.; Samson, L. D.; Sandilya, K.; Sly, P. D.; Smith, K. R.; Steiner, A.; Stewart, R. B.; Suk, W. A.; van Schayck, O. C. P.; Yadama, G. N.; Yumkella, K.; Zhong, M. The Lancet Commission on Pollution and Health. *Lancet* **2018**, *391* (10119), 462−512.

(9) World Health Organization. WHO Coronavirus (COVID-19) Dashboard. https://covid19.who.int (accessed 2022-05-29).

(10) Bolton, E. E.; Wang, Y.; Thiessen, P. A.; Bryant, S. H. PubChem: Integrated Platform of Small Molecules and Biological Activities. In *Annual Reports in Computational Chemistry*; Elsevier, 2008; Vol. *4*, pp 217−241. DOI: 10.1016/S1574-1400(08)00012-1.

(11) Kim, S.; Chen, J.; Cheng, T.; Gindulyte, A.; He, J.; He, S.; Li, Q.; Shoemaker, B. A.; Thiessen, P. A.; Yu, B.; Zaslavsky, L.; Zhang, J.; Bolton, E. E. PubChem in 2021: New Data Content and Improved Web Interfaces. *Nucleic Acids Res.* **2021**, *49* (D1), D1388−D1395.

(12) Pence, H. E.; Williams, A. ChemSpider: An Online Chemical Information Resource. *J. Chem. Educ.* **2010**, *87* (11), 1123−1124.

(13) Wishart, D. S.; Tzur, D.; Knox, C.; Eisner, R.; Guo, A. C.; Young, N.; Cheng, D.; Jewell, K.; Arndt, D.; Sawhney, S.; Fung, C.; Nikolai, L.; Lewis, M.; Coutouly, M.-A.; Forsythe, I.; Tang, P.; Shrivastava, S.; Jeroncic, K.; Stothard, P.; Amegbey, G.; Block, D.; Hau, D. D.; Wagner, J.; Miniaci, J.; Clements, M.; Gebremedhin, M.; Guo, N.; Zhang, Y.; Duggan, G. E.; Macinnis, G. D.; Weljie, A. M.; Dowlatabadi, R.; Bamforth, F.; Clive, D.; Greiner, R.; Li, L.; Marrie, T.; Sykes, B. D.; Vogel, H. J.; Querengesser, L. HMDB: The Human Metabolome Database. *Nucleic Acids Res.* **2007**, *35* (Database), D521−D526.

(14) Wishart, D. S.; Guo, A.; Oler, E.; Wang, F.; Anjum, A.; Peters, H.; Dizon, R.; Sayeeda, Z.; Tian, S.; Lee, B. L.; Berjanskii, M.; Mah, R.; Yamamoto, M.; Jovel, J.; Torres-Calzada, C.; Hiebert-Giesbrecht, M.; Lui, V. W.; Varshavi, D.; Varshavi, D.; Allen, D.; Arndt, D.; Khetarpal, N.; Sivakumaran, A.; Harford, K.; Sanford, S.; Yee, K.; Cao, X.; Budinski, Z.; Liigand, J.; Zhang, L.; Zheng, J.; Mandal, R.; Karu, N.; Dambrova, M.; Schiöth, H. B.; Greiner, R.; Gautam, V. HMDB 5.0: The Human Metabolome Database for 2022. *Nucleic Acids Res.* **2022**, *50* (D1), D622−D631.

(15) NORMAN Network. NORMAN Suspect List Exchange – NORMAN-SLE. https://www.norman-network.com/nds/SLE/ (accessed 2022-04-29).

(16) Schymanski, E. L.; Bolton, E. E. FAIR Chemical Structures in the Journal of Cheminformatics. *J. Cheminform* **2021**, *13* (1), 50.

(17) Schymanski, E. L.; Bolton, E. E. FAIR-Ifying the Exposome Journal: Templates for Chemical Structures and Transformations. *Exposome* **2021**, osab006.